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6425 Boaz Lane, Room G05
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The objective of this research project was to further develop and integrate numerical methods for the fast and accurate simulation of wave propagation problems in the time domain. In support of the long-term goal of creating high-quality software for simulating waves, we seek methods which are not only efficient, but which are reliable in that both their stability and the accuracy of the results are essentially guaranteed. In support of this goal we have developed: (i.) convenient implementations of optimal local radiation boundary sequences for isotropic waves, with implementations in a wide variety of popular discretization schemes for Maxwell's equations; (ii.) extensions of

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Final Report: Fast, Multiscale Algorithms for Wave Propagation in Heterogeneous Environments

ABSTRACT

The objective of this research project was to further develop and integrate numerical methods for the fast and accurate simulation of wave propagation problems in the time domain. In support of the long-term goal of creating high-quality software for simulating waves, we seek methods which are not only efficient, but which are reliable in that both their stability and the accuracy of the results are essentially guaranteed. In support of this goal we have developed: (i.) convenient implementations of optimal local radiation boundary sequences for isotropic waves, with implementations in a wide variety of popular discretization schemes for Maxwell's equations; (ii.) extensions of these sequences to more complex systems arising in linear elasticity; (iii.) new highly efficient energy-stable discretization schemes on structured grids - these include methods based on Hermite interpolation and compact difference schemes constructed using Galerkin techniques; (iv.) stable coupling of the efficient structured grid methods with upwind discontinuous Galerkin methods defined on unstructured grids - using hybrid grids allows us to treat very complex geometry with efficency comparable to simple domains; (v.) natural upwind discontinuous Galerkin discretizations for wave equations in second order form - using the second order form for complex systems results in fewer dependent variables.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received		Paper
01/04/2016	21.00	M. Beroiz, T. Hagstrom, S.R. Lau, R.H. Price. Multidomain, sparse, spectral-tau method for helically symmetric flow, Computers & Fluids, (10 2014): 0. doi: 10.1016/j.compfluid.2014.05.028
01/04/2016	23.00	Xi (Ronald) Chen, Daniel Appelö, Thomas Hagstrom. A hybrid Hermite–discontinuous Galerkin method for hyperbolic systems with application to Maxwell?s equations, Journal of Computational Physics, (01 2014): 501. doi: 10.1016/j.jcp.2013.09.046
01/04/2016	24.00	Thomas Hagstrom. High-resolution difference methods with exact evolution for multidimensional waves, Applied Numerical Mathematics, (07 2015): 114. doi: 10.1016/j.apnum.2014.07.001
01/04/2016	25.00	Daniel Baffet, Thomas Hagstrom, Dan Givoli. Double Absorbing Boundary Formulations for Acoustics and Elastodynamics, SIAM Journal on Scientific Computing, (01 2014): 1277. doi: 10.1137/130928728
01/04/2016	27.00	Daniel Appelo, Thomas Hagstrom. A new discontinuous Galerkin formulation for wave equations in second order form, SIAM J Numer Anal, (12 2015): 2705. doi:
08/31/2012	1.00	Ronald Chen, Thomas Hagstrom. P-adaptive Hermite methods for initial value problems, Mathematical Modeling and Numerical Analysis, (05 2012): 545. doi:
08/31/2012	11.00	Thomas Hagstrom. HIGH-ORDER RADIATION BOUNDARY CONDITIONS FORSTRATIFIED MEDIA AND CURVILINEAR COORDINATES, Journal of Computational Acoustics, (06 2012): 0. doi:
08/31/2012	10.00	Daniel Baffet, Jacobo Bielak, Dan Givoli, Thomas Hagstrom, Daniel Rabinovich. Long-time stable high-order absorbing boundary conditions for elastodynamics, Computer Methods in Applied Mechanics and Engineering, (10 2012): 20. doi:
08/31/2012	7.00	Daniel Appelo, Thomas Hagstrom. On Advection by Hermite Methods, Pacific Journal of Applied Mathematics, (05 2012): 0. doi:
08/31/2012	2.00	Thomas Hagstrom, George Hagstrom. Grid-stabilization of high-order one-sided differencing II. Second-orderwave equations, Journal of Computational Physics, (01 2012): 0. doi:
08/31/2012	3.00	Eliane Becache, Dan Givoli, Thomas Hagstrom, Kurt Stein. Complete radiation boundary conditions for convective waves, COMMUNICATIONS IN COMPUTATIONAL PHYSICS, (10 2011): 610. doi:
08/31/2012	4.00	Daniel Rabinovich, Dan Givoli, Jacobo Bielak, Thomas Hagstrom. A finite-element scheme with a high-order absorbing boundary condition for elastodynamics, Computer Methods in Applied Mechanics and Engineering, (06 2011): 2048. doi:
09/17/2013	16.00	Daniel Baffet, Jacobo Bielak, Dan Givoli, Thomas Hagstrom, Daniel Rabinovich. Long-time stable high-order absorbing boundary conditions for elastodynamics, Computer Methods in Applied Mechanics and Engineering, (05 2012): 241. doi:

09/17/2013 18.00 Daniel Rabinovich, Dan Givoli, Thomas Hagstrom, Jacobo Bielak . STRESS–VELOCITY COMPLETE RADIATIONBOUNDARY CONDITIONS,
Journal of Computational Acoustics, (04 2013): 1350003. doi:

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01/05/2016 33.00	Daniel Rabinovich, Dan Givoli, Jacobo Bielak, Thomas Hagstrom. The double absorbing boundary method forel astodynamics in homogeneous and layered media, Advanced Modeling and Simulation in Engineering Sciences, (04 2015): 0. doi:

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Number of Papers published in non peer-reviewed journals:

(c) Presentations

``A few things I learned from Herb Keller'', Keller/Isaacson Memorial Conference on Numerical Analysis, Courant Institute, New York, 2009.

``An Introduction to Radiation Boundary Conditions for Time-Domain Scattering Problems'', IMA PI Summer School on Computational Wave Propagation, Michigan State University, 2010.

``Complete Radiation Boundary Conditions: Theory and Application'', SIAM Annual Meeting, Pittsburgh, 2010.

``Complete radiation boundary conditions on rectangular domains'', AMS Midwest Sectional Meeting, Notre Dame, 2010.

``Approximate Radiation Boundary Conditions for Time-Dependent Waves'', Applied Inverse Problems, Texas A&M, 2011.

``Towards the Ultimate Solver for the Wave Equation in the Time Domain'', Applied Math and Imaging Sciences Workshop, UT Pan-American, 2011.

``Complete radiation boundary conditions'', Cambridge Workshop on Computational Wave Propagation, Isaac Newton Institute, Cambridge, UK 2010.

``HP-Refinement and DG Coupling for Hermite Methods'' 2011 Finite Element Rodeo, Texas A&M.

``Complete Wave Representations and Optimal Local Radiation Boundary Conditions'', SIAM Conference on Comptational Science and Engineering, Reno, 2011.

``Accurate Methods for Time-Domain Scattering'', SIAM Conference on Comptational Science and Engineering, Reno, 2011.

``Boundary conditions for simulating waves'', Eigenvalues/singular values and fast PDE algorithms: acceleration, conditioning, and stability, Banff International Research Station, Banff, CA 2012.

``Discretization methods for waves'', Nonlinear solvers for high-intensity focused ultrasound with application to cancer treatment, AIMS, Palo Alto, 2012.

``Hermite methods for aeroacoustics'', Acoustics 2012, Hong Kong.

``Hermite spectral elements'', Finite Element Rodeo 2012, Houston.

``Hermite methods for hyperbolic systems: Basic theory'', SIAM Conference on Computational Science and Engineering, Boston 2013

``Hybrid Hermite-DG Methods for Hyperbolic IBVPs'', Finite Element Rodeo, LSU 2013

``Towards the Ultimate Solver for Wave Equations in the Time Domain'', Forum on Scientific and Engineering Computing, Chinese Academy of Sciences, Beijing 2013

``Boundary conditions for high-resolution simulations of waves'', International Conference on Difference Schemes and their Applications, Moscow 2013

``Adaptive and hybridized Hermite methods for initial-boundary value problems'', MAFELAP 2013, London

``High-Order Energy-Stable Methods for Hyperbolic IBVPs on Structured-Unstructured Grids'', Finite Element Rodeo, Austin, TX 2014

``Dispersion and Dissipation of Hermite Methods in Multiple Dimensions'', C.-Y. Jang, Finite Element Rodeo, Austin, TX 2014

``High-resolution upwind methods for waves'', ICOSAHOM, Salt Lake City 2014

``Robust high-order methods for waves'', ICOSAHOM, Salt Lake City 2014 (Plenary Talk)

``Energy stable difference approximations to double absorbing boundary conditions'', K. Juhnke, ICOSAHOM, Salt Lake City 2014

``Multidimensional dissipation and dispersion analysis and Lp stability for Hermite methods'', C.-Y. Jang, ICOSAHOM, Salt Lake City 2014

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01/05/2016	37.00	Thomas Hagstrom. Radiation boundary conditions for time-domain scattering problems, Oberwohlfach Workshop on Computational Electromagnetism and Acoustics. 14-FEB-10, . : ,
01/05/2016	36.00	Fritz Juhnke, Thomas Hagstrom. A DG discretization of a Double Absorbing Boundary, Waves 2015. 20-JUL-15, . : ,
01/05/2016	35.00	John Lagrone, Thomas Hagstrom. Double Absorbing Boundaries for Finite Difference Time Domain Electromagnetics, Waves 2015. 20-JUL-15, . : ,
08/31/2012	5.00	Daniel Appelo, Matthew Inkman, Thomas Hagstrom, Tim Colonius. Recent progress on Hermite methods for aeroacoustics, 17th AIAA/CEAS Aeroacoustics Conference . 08-JUN-11, . : ,
08/31/2012	6.00	Thomas Hagstrom, Daniel Appelo, Chang Young Jang . HERMITE METHODS FOR HYPERBOLIC-PARABOLIC SYSTEMS, Waves 2011. 25-JUL-11, . : ,
08/31/2012	8.00	Chang Young Jang, Daniel Appelo, Tim Colonius, Thomas Hagstrom, Matthew Inkman. An Analysis of Dispersion and Dissipation Properties of Hermite Methods and its Application to Direct Numerical Simulation of Jet Noise, 18th AIAA/CEAS Aeroacoustics Conference. 04-JUN-12, . : ,
08/31/2012	12.00	Kurt Stein, Thomas Hagstrom. Complete Radiation Boundary Conditions: Corners and Edges, Waves 2011. 25-JUL-11, . : ,

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(d) Manuscripts

Received		Paper
01/05/2016	30.00	Daniel Appelo, Thomas Hagstrom. An energy-based discontinuous Galerkin discretizationof the elastic wave equation in second order form, Comput. Meth. Appl. Mech. Eng (07 2015)
01/05/2016	34.00	Charles Epstein, Leslie Greengard, Thomas Hagstrom . On the stability of time-domain integral equationsf or acoustic wave propagation, Discrete and Continuous Dynamical Systems (08 2015)
01/05/2016	32.00	Jeffrey Banks, Thomas Hagstrom . On Galerkin Finite Difference Methods, Journal of Computational Physics (08 2015)
08/31/2012	13.00	Seungil Kim, Thomas Hagstrom. COMPLETE RADIATION BOUNDARY CONDITIONS FOR THEHELMHOLTZ EQUATION I: WAVEGUIDES, Mathematics of Computation (06 2012)
09/17/2013	14.00	Daniel Baffet, Thomas Hagstrom, Dan Givoli. Double Absorbing Boundary Formulations for Acoustics and Elastodynamics, SIAM J Scientific Computing (08 2013)
09/17/2013	15.00	Xi Chen, Daniel Appelo, Thomas Hagstrom. A Hybrid Hermite - Discontinuous Galerkin Method forHyperbolic Systems with Application to Maxwell's Equations, Journal of Computational Physics (06 2013)
09/17/2013	20.00	Leslie Greengard, Thomas Hagstrom, Shidong Jiang. The solution of the scalar wave equation in the exterior of a sphere, Journal of Computational Physics (08 2013)
09/17/2013	19.00	Thomas Hagstrom, Dan Givoli, Daniel Rabinovich, Jacobo Bielak. The Double Absorbing Boundary Method, Journal of Computational Physics (05 2013)

TOTAL: **8**

Number of Manuscripts:

Books

Received   Book

TOTAL:

Received	Book Chapter
01/05/2016 28.00	Daniel Appelo, Thomas Hagstrom . Solving PDEs with Hermite Interpolation, Switzerland: Springer-Verlag , (12 2015)

TOTAL: 1

Patents Submitted

Patents Awarded

Awards

Ford Research Fellow, SMU

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Kurt Stein	1.00	
Chang-Young Jang	0.12	
John Lagrone	0.25	
Fritz Juhnke	0.25	
FTE Equivalent:	**1.62**	
Total Number:	**4**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Seungil Kim	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Thomas Hagstrom	0.13	
FTE Equivalent:	**0.13**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:...... 0.00

Names of Personnel receiving masters degrees

NAME	
John Lagrone	
Fritz Juhnke	
Total Number:	**2**

Names of personnel receiving PHDs

NAME	
Kurt Stein	
Chang-Young Jang	
Total Number:	**2**

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

Technology Transfer

We have had contact with a few businesses, primarily concerning the implementation of CRBCs in their codes. These include Hughes Research Lab, Schlumberger-Doll Research, Shell, and HyPerComp. In particular, we have provided both Hughes and HyPerComp with codes to compute optimal parameters, and we have also provided HyPerComp with our research codes which implement the method. A longer-term collaboration with HyperComp is being completed, funded by an STTR. Using this additional funding we have developed a library of implementations of the CRBCs. In particular, CRBCs can now be used with HyPerComp's HDPhysics code, which is extensively utilized for DOD applications. The work with Shell, done in collaboration with Prof. Tim Warburton, then on the faculty at Rice University, is focused on the implementation of CRBCs in a new DG-based code for solving VTI models of seismic waves. We have initiated collaborations with scientists at CASC, Lawrence Livermore National Laboratory, and RPI concerning the use of their software package Overture, which contains both the EM solver to which the CRBCs are being ported and a grid generation package, Ogen, which we plan to use. In addition we are working together on upwind difference methods. Lastly we have initiated collaborations with Lucas Wilcox and Jeremy Kozdon at the Naval Postgraduate School centered around software frameworks for adaptive, hybridized solvers.

Scientific Progress

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1 Introduction

The overall goal of this research is the development and application of efficient algorithms for solving wave propagation problems in the time domain, with a particular emphasis on problems in electromagnetism, elasticity, and aeroacoustics. The basic challenges in building such algorithms are rooted in the physical nature of waves themselves; their defining feature is the ability to propagate large distances relative to the wavelength, carrying information about their sources and the medium through which they have traveled. Thus typical wave propagation problems exhibit multiple spatiotemporal scales.

Two crucial components of the highly-efficient, general-purpose wave simulator we envision are

- Reliable, low-cost methods for truncating the computational domain in the near field, thus avoiding sampling the wave field throughout space;
- Robust, high-resolution volume discretizations providing guaranteed accuracy using minimal degrees-of-freedom per wavelength.

We have made substantial progress on both of these issues, as we will detail below.

2 Radiation Boundary Conditions and Integral Equations

Our recently-developed theory of complete radiation boundary conditions (CRBCs) solves a long-standing problem in computational wave propagation; namely how to truncate the domain in the vicinity of regions of interest in such a way that reflections from the computational boundary can be efficiently eliminated to any desired accuracy [26, 22, 7, 23, 9]. **CRBCs are the provably optimal method for achieving this in the case of isotropic waves**, including the scalar wave equation and Maxwell's equations. In particular, as proven in [26], we can guarantee an accuracy, ϵ, over a time interval, T, assuming a separation, δ, of scatterers and sources from the computational boundary using a CRBC with p auxiliary variables per field with

$$p \propto \ln\left(\frac{1}{\epsilon}\right) \cdot \ln\left(\frac{cT}{\delta}\right).$$

In this project we have developed full implementations of CRBCs for both exterior and waveguide problems in three space dimensions, devised a new formulation better suited to second order formulations and staggered-grid codes, extended their construction to elastic waves and stratified media, completed an open-source software library to enable their general use. In addition we have initiated a study of numerical methods and proper formulations of time-domain integral equations for scattering problems.

2.1 Implementation of CRBCs with Corners and Edges

As the major component of his doctoral thesis in computational mathematics at SMU, Kurt Stein, supporated as an RA on this project, completed the development and initial testing of a high-order, parallelized, $3+1$ dimensional structured grid solver for first order hyperbolic systems, with an implementation of CRBCs built in. The implementation uses grid-stabilized finite difference methods [24, 25] up through 12th order. The mathematical structure of CRBCs involves the evolution of a hyperbolic system of auxiliary variables defined only on the domain boundary. For example, along a boundary with normal in the $\mathbf{e_x}$ coordinate direction this auxiliary system takes the form:

$$A_0 \frac{\partial \mathbf{\Phi}}{\partial t} + A_y \frac{\partial \mathbf{\Phi}}{\partial y} + A_z \frac{\partial \mathbf{\Phi}}{\partial z} + \Sigma \mathbf{\Phi} = 0,$$

where $\mathbf{\Phi}$ is a vector of length $m(p+1)$ for a boundary condition order of p and a hyperbolic system with m independent variables. Here one set of m variables is the trace of the interior solution. To close this system boundary conditions are required at face edges. These in turn are provided by edge variables which satisfy their own auxiliary system. Finally the edge variables require boundary conditions at corners, which are provided by another set of auxiliary corner variables. Stein successfully implemented all of these coupled systems. His code achieves the *a priori* error estimates of [26]. We illustrate this in Figures 1-2. In the first case, a duct, the auxiliary system is closed using a physical boundary. In the second, free space, it is closed using the edge and corner systems.

2.2 Double absorbing boundary implementation of CRBCs

There are some restrictions and inconveniences with the implementation of CRBCs described above. In particular the formulation requires writing the system in terms of characteristic variables as well as the effective use of sparse matrix solvers (we have used SuperLU and Umfpack) to treat the corner and edge systems. The former issue is particularly felt when solving wave equations in second order form or when using the popular Yee scheme for Maxwell's equations. To deal with these issues we have developed an alternative formulation called the double absorbing boundary (DAB) [23, 9]. In the DAB we solve the auxiliary system for $\mathbf{\Phi}$ not on the boundary but in a thin (one element or one stencil width) layer near the boundary. The DAB does not require first order systems, characteristic variables, or semi-implicit systems at edges and corners. It is slightly more

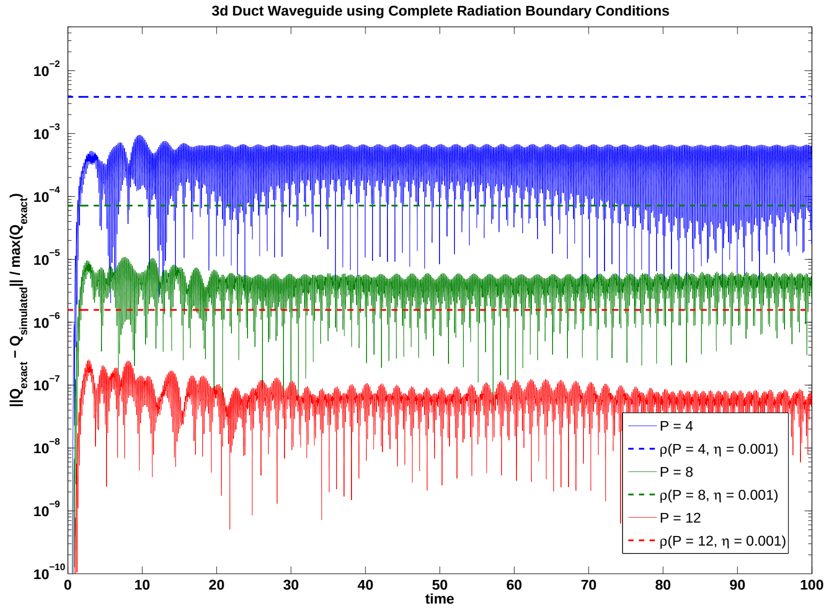

Figure 1: Maximum observed and predicted errors for solution of the acoustic system with $c = 1$ in a duct with square cross-section. Here the solution was produced by a point source at the origin, and simulated using 8th order differencing in space combined with 4th order Runge-Kutta time stepping. The duct width is 2 as is the width of the computational domain.

expensive than the original formulation in terms of flops, but requires less memory when edges and corners are present. It is being used in part of the software implementation of CRBCs discussed below.

2.3 Extensions to elastic waves and stratified media

The theoretical developments and implementations outlined above assume, in the far field, that the medium is homogeneous and isotropic and that there is a single wave speed. This is reasonable, for example, for studying electromagnetic scattering in a vacuum or a dielectric medium, but is not accurate for many problems arising, for example, in seismic wave studies. As such we have begun the process of extending the CRBCs to these more complex situations. In particular we have demonstrated excellent accuracy, even without full parameter optimization, for applications of the CRBCs to problems in stratified media as well as for some anisotropic problems [21, 7, 22]. This allows their application, for example, in layered waveguides and for advective acoustics.

We have also initiated their study for applications to elastic waves [8, 35, 34]. Complications with the elastic wave system include the presence of multiple wave speeds, boundary conditions involving oblique derivatives, and anisotropic media. In many cases stability is difficult to obtain; for example no known stable PMLs exist for certain orthotropic media [6]. We have shown that CRBCs applied to the elastic wave equation, with appropriate parameter choices, are always long-

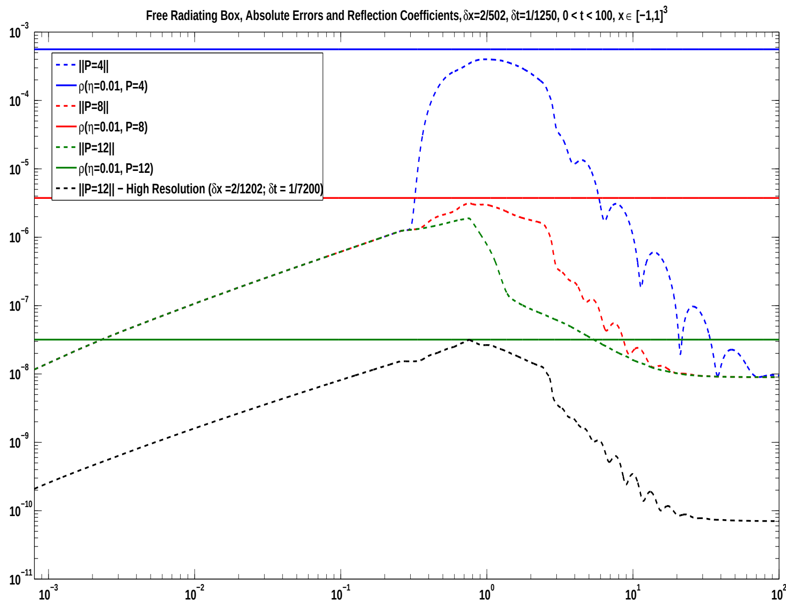

Figure 2: Maximum observed and predicted errors for solution of the acoustic system with $c = 1$ for a solution in free space produced by a point source at the origin, and simulated using 8th order differencing in space combined with 4th order Runge-Kutta time stepping. The width of the computational domain is 2.

time stable. This is in contrast with all other high-order radiation conditions which have been proposed for elastic waves which suffer from long-time error growth. We illustrate this in Figure 3 below.

We are actively working on improving these extensions. The fundamental issue, being studied by a Ph.D. student, John Lagrone, who has been funded as an RA on this project as well as on a related STTR, is the computation of optimal parameters and an estimate of convergence with increasing boundary condition order. This is important not only for elastic wave models but also for electromagnetic waves in more complex media such as metamaterials. He is also looking into more general formulations in case they are needed to produce efficient methods for arbitrary wave systems.

2.4 A CRBC Software Library

In work with HyPerComp, primarily funded by an STTR but also partially supported by this grant, we have developed an open source software library, **rbcpack** (www.rbcpack.org), with implementations of CRBCs for various volume discretizations of Maxwell's equations. The library generally involves a preprocessor which computes optimal parameters given ϵ, c, T, and δ, sets up the auxiliary system, and provides an interface to the volume solver. Currently two pieces to the library are complete or nearly complete. The first is the implementation in the popular Yee scheme, developed

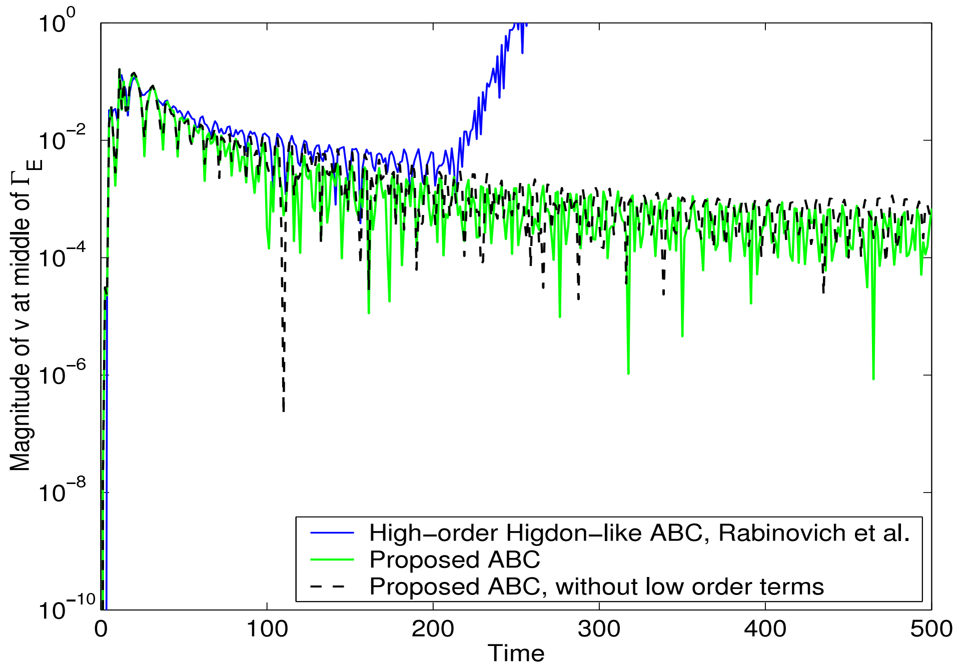

Figure 3: The magnitude of a solution component for a simulation of transversely 1-periodic elastic waves in $2+1$ dimensions. The solution displaying long-time instability was obtained using the traditional implementation of high-order radiation boundary conditions as first proposed by Higdon. The long-time stable solutions were produced using our new CRBC formulation but different parametrizations.

by John Lagrone and utilizing the DAB formulation. This has been completely tested with our own codes and extensively documented; it will be released once our first external users verify that it can be linked easily as a library. The second is a boundary-based implementation for arbitrary-order discontinuous Galerkin discretizations. This has been completely tested for hexahedral grids and for tetrahedral grids in waveguides. Once the implementation on tetrahedral grids for exterior problems is complete, which we expect soon, this code will also be released. It can be used in conjunction with HyPerComp's HDPhysics platform. The third component is a DAB implementation for high-order difference approximations to second order formulations with Overture's cgmx code as a target application. Currently a two-dimensional version of the code, developed by Fritz Juhnke, a doctoral student who was supported as an RA on this project and the related STTR, is being coupled with cgmx; he has successfully tested it using a home-grown version of the 6th order space-time approximation native to cgmx. Once this coupling is proven to work he will move on to the three-dimensional implementation. Note that with a DAB formulation extensions from two to three space dimensions do not require conceptually distinct discrete systems, so it is reasonable to expect that the extension will be complete in less than a year.

2.5 Time-domain integral equations for electromagnetic scattering

An alternative to the volume-based methods we work on for simulating electromagnetic waves are methods based on integral equations. These have the advantage that no volume grid is required, so that scattering from extremely complex structures (e.g. circuit boards) can be carried out without the need for a costly grid generation step. This approach has been reinvigorated in the past decade by the introduction of the so-called Plane Wave Fast Time Domain Algorithm (PWFTD) [16, 36], which is a time-domain version of Greengard and Rokhlin's celebrated fast multipole algorithm. However, the theory behind these equations and the algorithms used to solve them is not well developed, and a number of seemingly attractive discretization techniques experience unexplained instabilities. Our first goal is to develop more efficient time-stepping procedures for these unusual equations. By studying the simple problem of scattering from a sphere we have established a connection between these time-domain equations and neutral delay differential equations, and have developed stable explicit methods. In addition we have shown how to alter the integral equation so that the decay properties of the potentials match those of the physical fields. This is joint work with Leslie Greengard of the Simons Foundation and the Courant Institute and Charlie Epstein of the University of Pennsylvania [15]. In Figure 4 we illustrate the remarkably different long time behavior of the density for different formulations of the same scattering problem. Note that the solution of the wave equation itself decays exponentially.

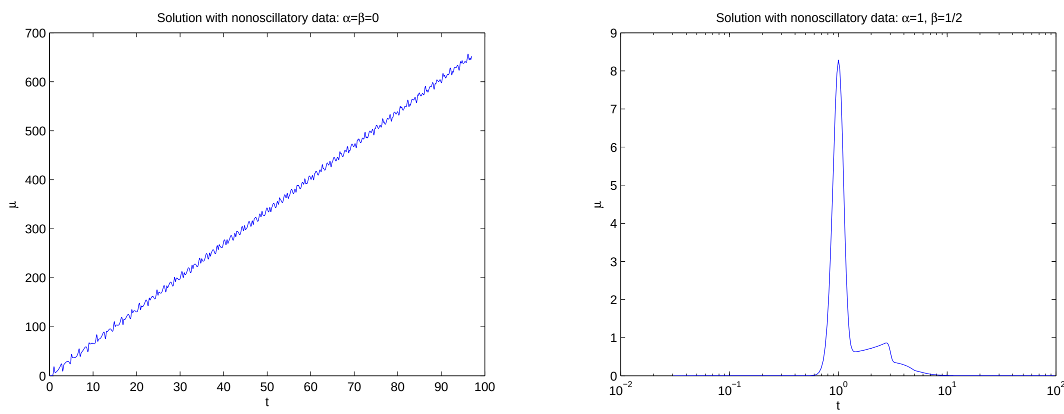

Figure 4: Density $\mu(t)$ at mode 0 for scattering of a plane Gaussian pulse from a sphere. On the left the solution using the standard single layer potential and on the right an appropriately chosen combined field representation. We use an explicit multistep method of order 6.

In addition we have developed codes for the accurate evaluation of exact solutions for both scalar wave and electromagnetic scattering from a sphere [18, 19]. These provide benchmark solutions for any time-domain scattering solver.

2.6 Frequency domain applications

Although the primary focus of our boundary condition development is the time-domain, the CRBCs can also be used for problems posed in the frequency domain. This development was led by Dr. Seungil Kim, who for two years was a postdoctoral fellow supported by the grant. The basic mathematical formulation and the theory of finite element approximations is worked out in [30, 31]. In particular in [31] we are able to provide a complete mathematical justification for the edge and corner closure conditions, which as yet are unavailable in the time domain.

Besides the domain truncation itself, CRBCs can be used in place of PMLs to develop sweeping preconditioners, as first proposed by Engquist and Ying [14]. These address one of the most important issues for frequency domain compuations, namely the efficient solution of the resulting algebraic system. In particular it is argued in [14] and elsewhere that sweeping preconditioners can deliver optimal or near-optimal convergence rates. Kim has shown that CRBCs are an effective replacement for PML in this context [32]. We note that the CRBCs have also been similarly used to develop improved parabolized models of jet noise by Towne and Colonius [39, 40].

The criteria for optimizing the CRBC parameters for use in a sweeping preconditioner differ somewhat from those in the radiation boundary condition problem, and in any case most applications involve variable coefficients where optimal parameters are unknown. Lagrone has done some work to use rational Krylov methods (e.g. [33]) to construct locally optimized transmission conditions. We expect to return to this development in the future.

3 Energy-stable high-resolution volume discretizations

Our belief is that to best exploit advances in computing technology, algorithms based on high-order space-time discretizations are needed. The reasons for this are two-fold:

i. One aims to solve more difficult problems as measured by the number of wavelengths over which accuracy must be maintained, and in the treatment of heterogeneous media with disparate physical properties. More simply put, one wishes to solve problems exhibiting multiple spatiotemporal scales. Due to their minimal dispersion error, high-order methods require orders of magnitude fewer degrees-of-freedom than traditional lower order schemes when the number of wavelengths propagated becomes large, and thus they are a natural choice for challenging problems.

ii. Higher order methods generally involve more localized computation than their lower order counterparts. Thus they exhibit larger computation-to-communication ratios and can therefore better exploit modern multicore architectures.

The main challenges to realizing the potential of high-order discretizations are to develop methods which are robustly stable and capable of dealing with complex geometric features. For unstructured meshes, upwinded discontinuous Galerkin (DG) methods [27] are an excellent choice which we employ. In particular they are energy-stable and applicable on very general meshes. The downside of DG methods, or more generally any element-based methods, is artifically stiff derivative operators. (See, e.g., [42].) The effect of this artificial stiffness is the need to take small times steps, which has essentially limited most methods to less-than-optimal orders. For polynomial-based discretizations the only way to avoid this artificial stiffness is to avoid differentiation throughout the polynomial's domain of definition, which is best achieved by using structured grids. Thus we are focused on the use of hybrid structured-unstructured grids, combining upwind DG discretizations with energy-stable structured grid methods which allow large time steps throughout much of the domain. We are studying two distinct methods of this type: novel spectral elements based on Hermite interpolation [17, 5], and compact difference methods derived from DG ideas [10]. In addition we have developed new upwind DG methods for wave equations in second order form.

3.1 Hermite Methods

Hermite methods are spectral element methods with unique properties which make them ideal for efficient implementation on modern multicore architectures, a project underway in collaboration with Warburton and his group [41]. In comparison with existing techniques, they allow the **independent evolution of thousands of degrees-of-freedom** over relatively large time steps, effectively minimizing communication requirements. In particular, the only time step restriction is the physical CFL condition independent of order. Thus for methods of order 10 or more the method is at least 10 times faster than standard DG, and has much better (essentially optimal) computation-to-communication characteristics.

Hermite methods are energy-stable, but the analysis requires the introduction of an unusual energy based on high-order derivatives. Precisely, for methods of order $2m+1$, we prove stability using the seminorm:

$$|u|^2_{[m+1]} \equiv \int_\Omega \left(\prod_j D_j^{m+1} u \right)^2 .$$

This leads to theoretical barriers to proving the stability for coupling with standard DG schemes on hybrid grids. Nonetheless we do have experimental verifications of the stability of hybridized Hermite-DG methods [11]. As an example, we have solved the TM Maxwell system on a disk using the hybrid grid shown in Figure 5, with convergence results for our 9th order implementation tabulated in Table 1. Of note, besides the fact that convergence at design order is observed, is the ratio of the time steps - in the extreme case we take 80 steps in each DG cell for every step in a Hermite cell. Analyzing the stability of the hybrid method is a priority for future research.

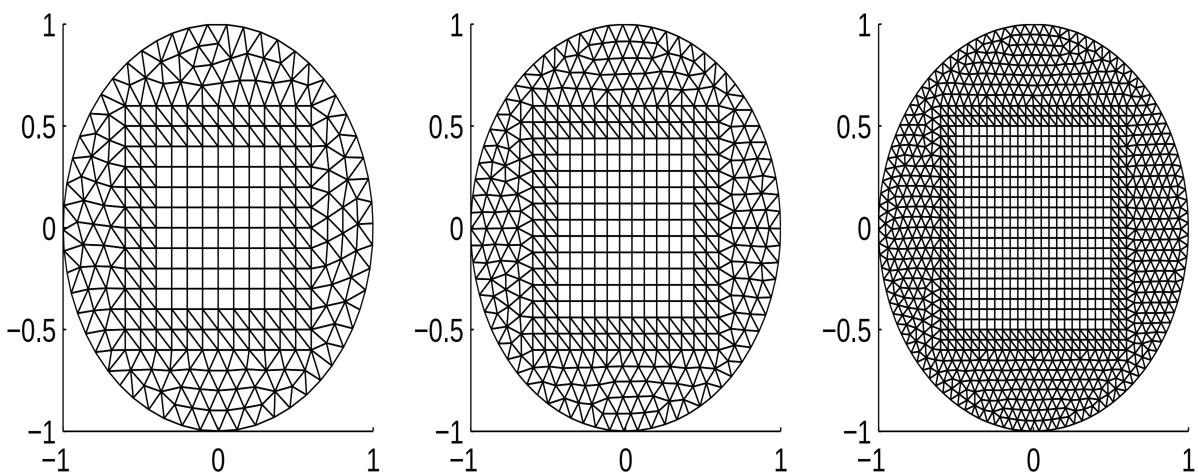

Figure 5: Hybrid grids used for a coupled Hermite-DG solver for Maxwell's equations. We use the DG scheme on the mapped triangular elements near the PEC boundary and the Hermite scheme elsewhere.

h	K	CFL	Δt_{DG}	Error	rate
0.1	447	0.7	1.83(E-03)	1.37(E-08)	
0.08	666	0.7	8.56(E-04)	1.42(E-09)	10.1
0.05	1525	0.7	4.09(E-04)	1.68(E-11)	9.4

Table 1: Experimental convergence for the hybrid Hermite-DG Maxwell solver on a disk.

In a series of papers we have examined the basic properties of Hermite methods, including their performance for nonsmooth solutions [2] and their dispersion/dissipation characteristics [28, 29]. The latter work was a central component of Chang-Young Jang's doctoral thesis; Dr. Jang received some RA support from the grant while he was a student. We note that the performance of the methods for propagating discontinuous solutions is particularly impressive. Interestingly it improves with increasing order; see Figure 6 below for comparisons with a WENO scheme [37]. We currently have no theory which fully explains this excellent behavior, but hope to develop one in the future. We also note that versions with full shock-capturing capabilities are being developed by our collaborator Appelö and his student Kornelus.

Additional work includes the implementation of a p-refinement strategy [12] and the outlines of a scheme for h-refinement on octrees [1]. From the theoretical perspective we need to prove stability for the p-refinements. We also need to develop an effective strategy for choosing between the two approaches.

Lastly, in collaboration with Daniel Appelö of UNM, we are about to release a basic open-source library, **CHIDES** (www.chides.org), to help explain Hermite methods and enable their wider use.

3.2 Galerkin Difference Methods

High-order difference methods provide a simple alternative to Hermite methods as a structured-grid solver. Recently, methods with the summation-by-parts (SBP) property have been incorporated into many unsteady aerodynamics simulators due to their guaranteed stability on poor grids [38]. However, a defect of existing high-order SBP methods is severe loss of accuracy at boundaries. Galerkin difference methods simply use the local piecewise polynomial bases associated with standard difference schemes in a Galerkin framework. They are closed at boundaries either using extrapolation to ghost points or by leaving the basis functions associated with ghost points in the Galerkin basis. In [10] we show that **the resulting compact difference schemes are superconvergent, like their DG counterparts, but have essentially order-independent time step stability restrictions** just as central difference methods possess when there are no boundaries. See, for example, Table 2 for the extremely slow growth with p of the eigenvalues of the differentiation matrices including the boundary closures. Additionally, although the mass matrices are not diagonal, they are tensor products of banded matrices and thus can be inverted with linear cost.

As they are based on the Galerkin framework, stable hybridization with standard DG methods on hybrid grids is automatic.

The Galerkin difference methods have both advantages and disadvantages relative to Hermite schemes. On standard architectures they are somewhat more efficient in terms of flops, but their communication patterns are not as ideal. We are just starting to experiment with the schemes, so

p	3	5	7	9	11	13	15	17
$\Delta x \cdot \rho(D^{p,G})$	2.02	2.17	3.41	3.18	3.67	3.81	3.57	3.84
$\Delta x \cdot \rho(D^{p,X})$	2.02	2.17	2.27	2.33	2.39	2.43	2.46	2.49

Table 2: Table of maximum eigenvalues and normalized stability constraint for first derivatives with the ghost, G, and extrapolation, X, basis closures at various orders. Here p is the method design order and D^p is the first derivative matrix including boundary conditions.

the development of more serious multidimensional implementations is a subject for future work, being carried out in collaboration with Jeff Banks of RPI. In particular we are also considering embedded boundary formulations which would enable the solution of problems in complex geometry on purely Cartesian grids.

3.3 Upwind DG methods for second order wave equations

In many cases second order formulations of wave equations have advantages over first order formulations. However, in our view the usual DG schemes for wave equations in second order form such as SIPDG [20] and LDG [13] are less attractive than their first order counterparts due to the lack of a natural upwinding strategy. In joint work with Appelö [4] **we propose a new, and quite general, formulation of DG methods for wave equations in second order form**, with applications to elastic waves demonstrated in [3]. The essential ideas behind the method are:

i. Introduce a weak approximation, $\mathbf{v}$, to the time derivative of the solution, $\mathbf{u}$.

ii. Build fluxes based on the Lagrangian form.

Precisely, consider a system with a potential energy function $G(\mathbf{u}, \nabla \mathbf{u}, \mathbf{x})$. Then the weak form on an element Ω_j is given by:

$$\begin{aligned}
\int_{\Omega_j} \left(\sum_k \frac{\partial G}{\partial u_{i,k}}(\phi_u, \nabla\phi_u, \mathbf{x}) \frac{\partial}{\partial x_k} + \frac{\partial G}{\partial u_i}(\phi_u, \nabla\phi_u, \mathbf{x}) \right) \left(\frac{\partial u_i^h}{\partial t} - v_i^h \right) &= \\
\int_{\partial\Omega_j} \sum_k n_k \frac{\partial G}{\partial u_{i,k}}(\phi_u, \nabla\phi_u, \mathbf{x}) \left(v_i^* - v_i^h \right), & \\
\int_{\Omega_j} \phi_{v,i} \frac{\partial v_i^h}{\partial t} + \sum_k \frac{\partial \phi_{v,i}}{\partial x_k} \frac{\partial G}{\partial u_{i,k}}(\mathbf{u}^h, \nabla\mathbf{u}^h, \mathbf{x}) + \phi_{v,i} \frac{\partial G}{\partial u_i}(\mathbf{u}^h, \nabla\mathbf{u}^h, \mathbf{x}) - \phi_{v,i} f_i(\mathbf{x}, t) &= \\
\int_{\partial\Omega_j} \sum_k n_k \phi_{v,i} w_{i,k}^*, &
\end{aligned}$$

where v_i^* and $w_{i.k}^*$ are appropriately chosen fluxes. Although the formulation may look complex, its implementation is fairly straightforward, and for complex systems it uses significantly fewer unknowns than LDG. In [4] we observe optimal convergence for both dissipative upwind fluxes and energy-conserving alternating fluxes. We also prove optimal convergence in the energy norm for simple cases.

The method is naturally formulated for any system in Lagrangian form, and we have experimented with it for various nonlinear model problems. These often develop singularities, and an interesting open problem is to develop conditions on discretization schemes which guarantee convergence to physically relevant weak solutions. We also note that the new formulation can be used to derive Galerkin difference methods which can be applied on hybrid grids. These issues will be a focus of our continued research into these methods.

4 Applications

Although our overall concentration is on the development of general-purpose algorithms for waves, we are interested in applications to challenging problems. One example is the simulation of seismic waves. This is particularly relevant for modeling earthquakes, but is also important for problems related to imaging underground geology. For the former problem we are collaborating with Jacobo Bielak of Carnegie Mellon University and Dan Givoli of the Technion. We have both Hermite and DG elastic wave codes, and a Galerkin difference elastic code is planned, but we need to look at their hybridization near geologic features in the earth's interior. Developing this code and applying it to basic benchmark problems will be a next step. We note that similar ideas can be used in the context of nondestructive evaluation.

In collaboration with Daniel Appelö of the University of New Mexico and Tim Colonius of Caltech we have developed a Hermite-based compressible Navier-Stokes solver. A major application, primarily funded by the NSF but benefiting from the work done under this grant, is the direct numerical simulation of jet noise at Reynolds numbers an order of magnitude higher than those attained previously, to within one order of magnitude of the Reynolds numbers where most relevant experiments are performed. The code is fully parallelized and we have carried out a number of experiments with turbulent compressible flows to verify its accuracy. As we complete some of our higher Reynolds number runs, we face the problem of extracting useful insights from the results. Here we hope to leverage work in model reduction, control theory, and data mining to use our simulations to develop better models of noise production.

Lastly we note that we expect HyPerComp to make extensive use of our radiation boundary condition library to solve problems in electromagnetism and acoustics of direct interest to the DOD.

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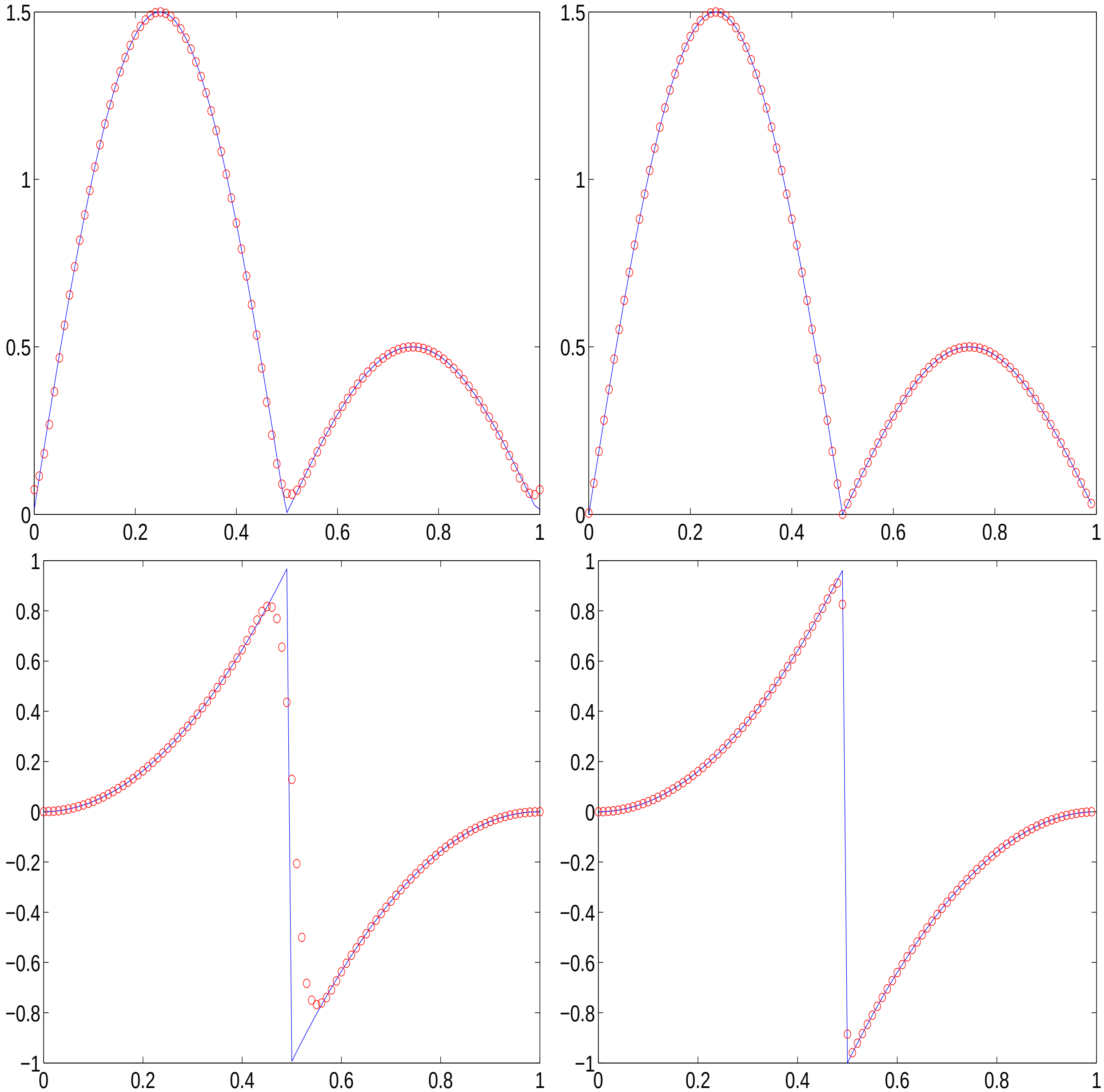

Figure 6: Comparison of a 5th order WENO scheme (left) with an 11th order Hermite scheme (right) for the linear advection of nonsmooth profiles. (The grid size for the WENO scheme is $\Delta x = \frac{1}{100}$ and for the Hermite scheme it is $\Delta x = \frac{1}{70}$.) We display the solutions after the profiles have propagated a distance of 1. For the discontinuous profile it is evident that the Hermite scheme produces a sharper front, but is also not oscillatory. Looking closer at the corners for the first profile, we also see some smearing of the WENO solution but none with Hermite. Note that we are using the base Hermite method with no enhancements to handle nonsmooth solutions.

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